

Catalysis Science with Hard X-rays

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NSLS-II Chemical and Energy Science Workshop
February 1, 2008

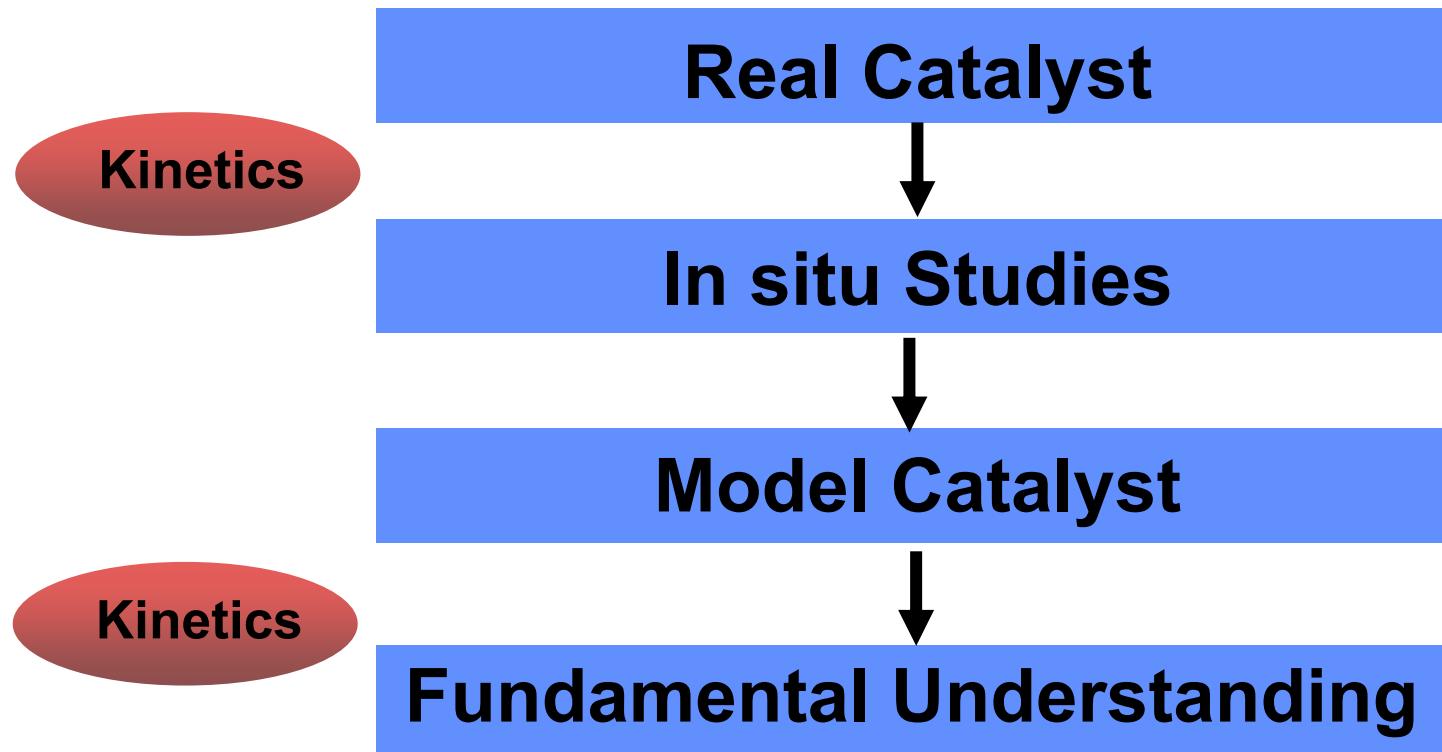


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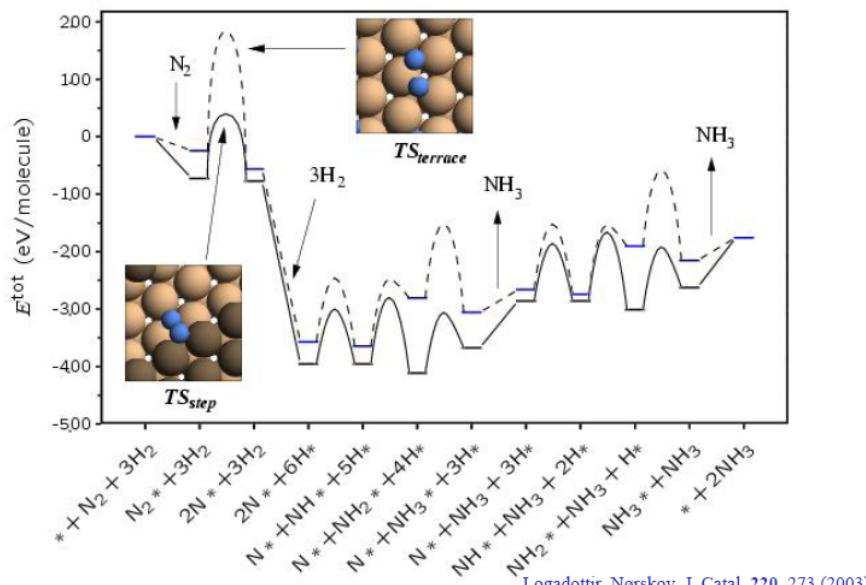
Understanding of Catalysis

- Basis of strategy is that knowledge of the structure of the reacting catalyst must be known in order to perform meaningful functional studies (kinetic experiments)



Understanding of Catalysis

- Final outcome of strategy is **FUNDAMENTAL UNDERSTANDING**.
- This results in a quantitatively correct microkinetic model of the system.
- Fundamental knowledge can be used for developing new and alternative catalysts.



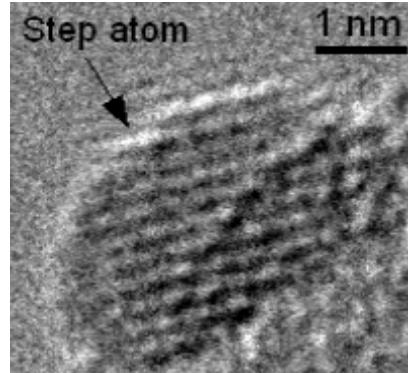
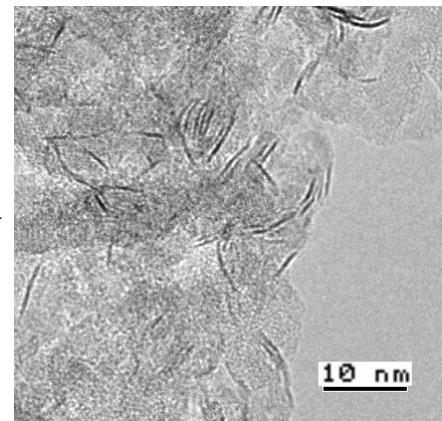
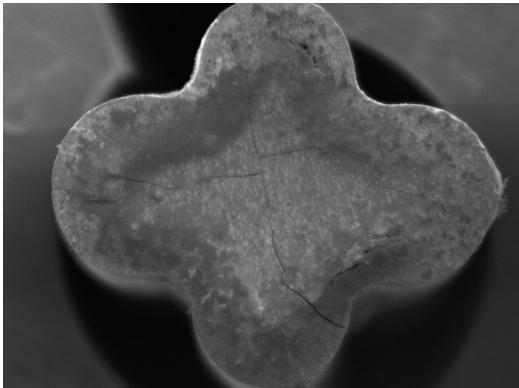
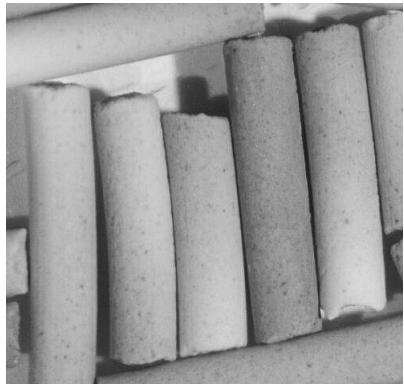
Logadottir, Nørskov, J. Catal. 220, 273 (2003)

Understanding of Catalysis

- Key feature of the strategy is that a suite of complimentary in situ analytical techniques are available to probe the geometric and electronic structure of the working catalyst.
- Each in situ experiment ideally requires the simultaneous detection of catalytic activity to allow quantitative correlations to be established.
- Hard X-rays are critical tool in this strategy:
 - Absorption
 - Scattering
- Ideally all techniques should be applicable to model and real catalyst systems

Real Catalyst Complexity

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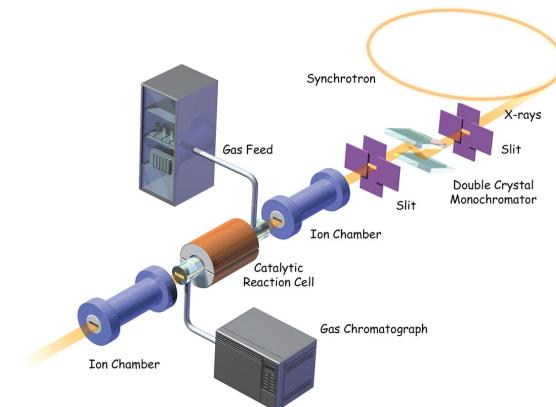
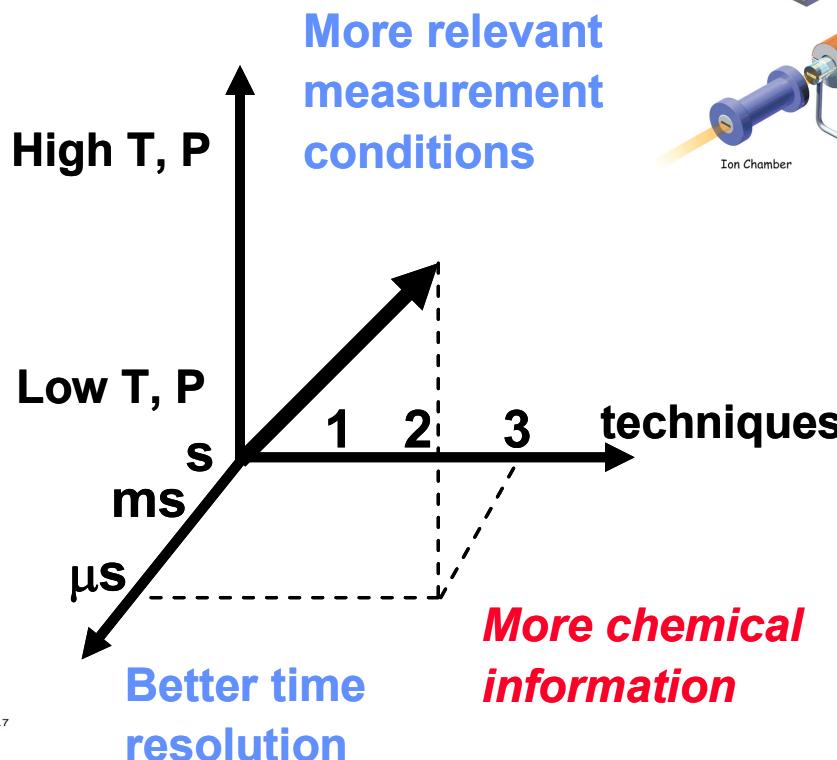
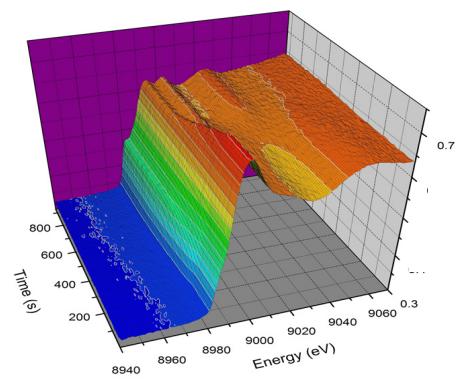


- **Information needed on many different length scales, elemental concentration, time scales.**

Roadmap for in situ Spectroscopy: Measurement Science

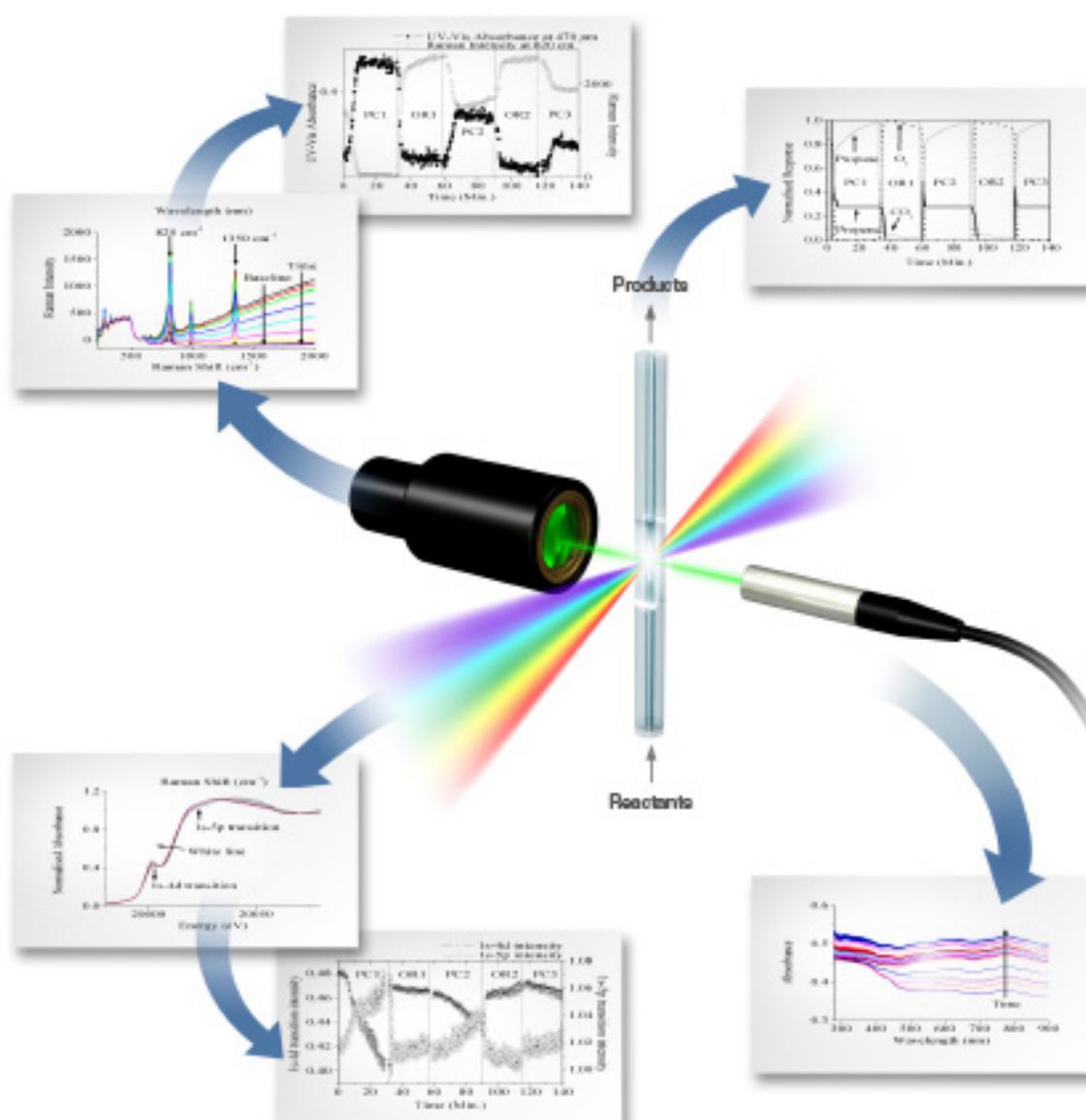
Improvements in spatial, temporal,
energy resolution

- Dynamics



Multi-technique time-resolved *in situ* characterization

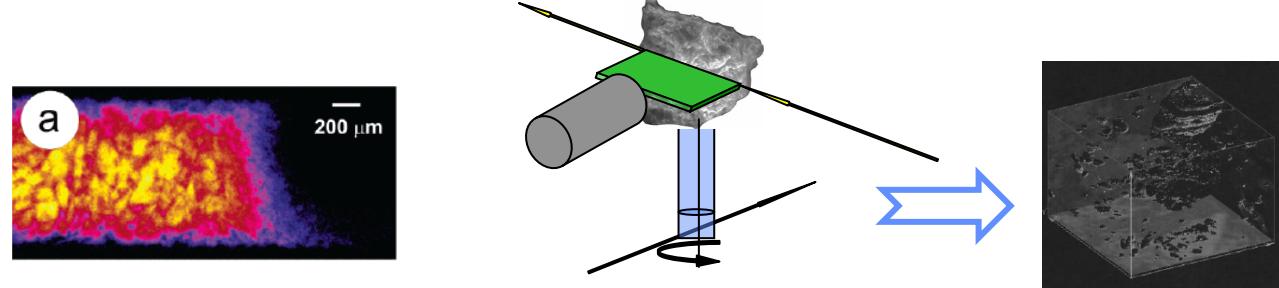
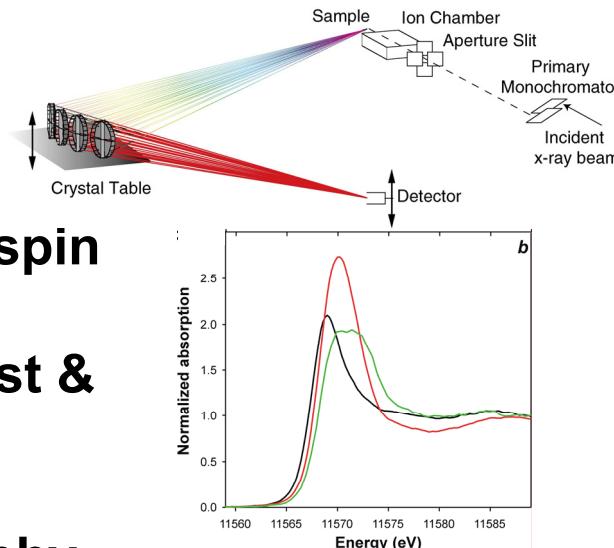
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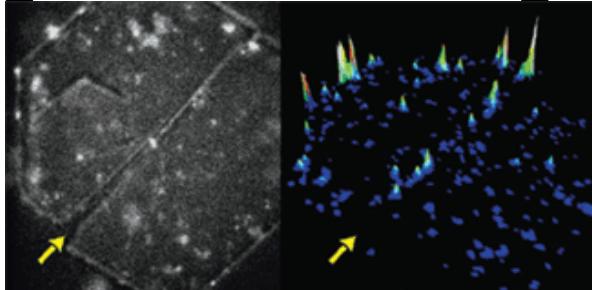
Synchrotron-based Real Time in situ Characterization

- Expanding capability, increasing complexity

- Selective XAS (High resolution fluorescence detection): valence selective, edge selective, spin selective....
- Adsorption site from XAFS: combining catalyst & adsorbent
- Spatial resolution / imaging – see recent NAS study “Visualizing Chemistry”: nanotomography with chemistry.



- Single molecule imaging at active site



Mapping the spatial distribution of active sites over a single catalytic crystal
(*fluorescence microscopy*)

M.B.J. Roeffaers, et al, Nature 2006, 439, 572

Spectroscopy (XAFS)

Time
Resolution

Automation

Sensitivity

Spatial
Resolution

**Spectroscopy
(XAFS)**

In situ

Energy
Resolution

Combined
Techniques

Enhanced S/N

Imaging